

ABSTRACT

004431469 : 110109
5 The present invention relates to crystallized
molecules and molecular complexes which comprise the
active site binding pocket or the FKBP12/FK506 binding
pocket of calcineurin or close structural homologues to
either binding pocket. This invention also relates to a
data storage material encoded with the corresponding
structure coordinates of those crystallized molecules or
molecular complexes. Such data storage material is
10 capable of displaying such molecules and molecular
complexes as a graphical three-dimensional representation
on a computer screen. In addition, this invention
relates to methods of using the structure coordinates of
those molecules or molecular complexes to solve the
15 structure of homologous proteins. This invention also
relates to methods of using the structure coordinates to
screen and design compounds that bind to calcineurin or
homologues thereof.